

Global Calculation of Nuclear Shape Isomers

Peter Möller (T-16), Ragnar Bengtsson and Peter Olivius (Lund University, Sweden);
moller@lanl.gov

Nuclear isomer states are long-lived states that often significantly impact various reaction rates in weapons environments.

The reaction rates on isomers are often challenging to measure. As a result many important rates are insufficiently known from experimental work; modeling them is therefore an important task.

We have previously reported that we have enhanced our model for calculating the potential energy of nuclei as a function of shape to also allow the study of axially asymmetric shapes. This is important both for modeling fission barriers of actinide nuclei and for modeling the structure of the nuclear ground state.

We report here on our use of the enhanced model for systematic, global calculations of the potential energy in the vicinity of the nuclear ground state for 7206 nuclei from ^{16}O to $A = 290$ from very proton-rich nuclei to very neutron-rich nuclei, for the following 3D grid of nuclear shapes: $\epsilon_2 = 0.0(0.025)0.45$, $\epsilon_4 = -0.12(0.02)0.12$, and $\gamma = 0(2.5)60$. In Fig. 1 we show as an example the calculated results for 12 different even-even nuclei. As is customary we display the calculated potential energy as a function of ϵ_2 and γ with ϵ_4 varying in the radial direction and γ in the angular direction. In each point the energy has been minimized with respect to the third shape-degree of freedom, ϵ_4 . In general this procedure will not yield a 2D surface that correctly describes the significant structures of the higher-dimensional space. However, we have found, by employing an imaginary water-immersion technique to analyze the full 3D space, that the saddles and minima in the 2D surfaces presented here correctly reflects the 3D structure. Our deformation coordinates are such that $\gamma = 0$ represents prolate nuclei and $\gamma = 60$ represents oblate nuclei. The tip of the “pie” corresponds to spherical shape. The energy is plotted in

Table 1—
Table of potential-energy minima for nuclei for which at least two minima are found. The higher minima are shape-isomers. The optimal saddle points between all pairs of minima are also tabulated, as well as the values of the three shape coordinates associates with the minima and saddle points. Here we list a small section of the complete results of the global calculation, which is about 60 pages. The right column, labeled S.H., gives the saddle point height relative to the higher of the pair of minima tabulated on this line.

Nucleus		Minimum				Saddle				Minimum				S.H.
N	A	ϵ_2	ϵ_4	γ	E (MeV)	ϵ_2	ϵ_4	γ	E (MeV)	ϵ_2	ϵ_4	γ	E (MeV)	E_{sad} (MeV)
Z = 39 (Y)														
44	83	0.225	0.06	50.0	3.23	0.100	0.02	60.0	3.51	0.000	0.00	0.0	3.18	0.28
60	99	0.275	-0.02	60.0	4.56	0.275	0.00	45.0	4.82	0.325	0.00	0.0	2.28	0.26
68	107	0.250	0.06	60.0	3.99	0.300	0.06	45.0	4.21	0.325	0.06	0.0	1.93	0.22
72	111	0.225	0.06	52.5	2.90	0.225	0.04	32.5	3.16	0.300	0.08	0.0	2.19	0.25
73	112	0.200	0.06	45.0	2.55	0.250	0.06	12.5	2.75	0.325	0.06	0.0	2.34	0.20
91	130	0.225	-0.06	0.0	1.62	0.200	-0.04	17.5	1.94	0.100	-0.02	30.0	1.49	0.32
		0.225	-0.06	0.0	1.62	0.200	-0.04	17.5	1.94	0.150	-0.02	52.5	1.48	0.32
		0.100	-0.02	30.0	1.49	0.125	-0.02	32.5	1.72	0.150	-0.02	52.5	1.48	0.24
Z = 40 (Zr)														
33	73	0.250	0.04	50.0	2.91	0.300	0.04	27.5	3.19	0.300	0.06	0.0	2.91	0.28
34	74	0.250	0.04	60.0	3.13	0.325	0.04	30.0	3.50	0.325	0.08	0.0	2.96	0.38
35	75	0.275	0.04	57.5	3.54	0.300	0.06	32.5	4.04	0.325	0.06	0.0	3.03	0.50
36	76	0.275	0.06	60.0	3.79	0.325	0.04	35.0	4.25	0.350	0.06	0.0	2.68	0.46
37	77	0.200	0.06	60.0	4.07	0.325	0.04	37.5	4.54	0.350	0.06	0.0	2.42	0.46
38	78	0.200	0.06	60.0	4.01	0.300	0.06	37.5	4.52	0.375	0.08	0.0	1.95	0.51
39	79	0.200	0.06	60.0	4.06	0.300	0.06	37.5	4.58	0.375	0.08	0.0	1.83	0.52
40	80	0.000	0.00	0.0	4.55	0.075	0.02	60.0	4.77	0.200	0.06	60.0	3.81	0.22
		0.000	0.00	0.0	4.55	0.075	0.02	60.0	4.77	0.375	0.08	0.0	2.00	0.22
		0.200	0.06	60.0	3.81	0.300	0.06	37.5	4.38	0.375	0.08	0.0	2.00	0.57
41	81	0.200	0.06	60.0	3.79	0.275	0.06	40.0	4.25	0.400	0.08	0.0	2.51	0.46
42	82	0.000	0.00	0.0	4.02	0.075	0.00	60.0	4.34	0.225	0.08	60.0	3.44	0.32
		0.000	0.00	0.0	4.02	0.075	0.00	60.0	4.34	0.375	0.08	0.0	2.98	0.32
		0.225	0.08	60.0	3.44	0.275	0.06	37.5	3.88	0.375	0.08	0.0	2.98	0.43
43	83	0.025	0.00	47.5	3.99	0.100	0.02	60.0	4.21	0.375	0.08	0.0	3.51	0.23
		0.025	0.00	47.5	3.99	0.100	0.02	60.0	4.21	0.225	0.08	57.5	3.35	0.23
		0.375	0.08	0.0	3.51	0.350	0.06	7.5	3.79	0.225	0.08	57.5	3.35	0.29
44	84	0.000	0.00	0.0	3.09	0.100	0.02	60.0	3.40	0.225	0.08	60.0	2.97	0.32
45	85	0.225	0.08	60.0	2.76	0.100	0.02	60.0	3.00	0.000	0.00	0.0	2.72	0.24

MeV, with $\dots -1, 0, 1, \dots$ MeV given by thick lines. The spacing between the thin lines is 0.2 MeV.

Several of the calculated potential-energy surfaces exhibit more than one minimum. In such surfaces we have indicated the minima with a dot and saddle points between all combinations of minima with crossed lines. For such nuclei we also tabulate pairwise all minima and the optimal saddle point between all pairs of minima and the associated shape parameters. A section of the global table is shown in Table 1. We plan to make the complete set of results, namely all contour surfaces, and a computer-readable

version of the full table available on the T-16 web site.

Many nuclear properties are affected if shape isomers are present in nuclei. For example, in nuclear β -decay the decay can proceed both to states in the lowest minimum, the nuclear ground state, and to states in the shape isomer. In neutron-induced reactions the reaction rates can be affected by the presence of a shape isomer. The availability of our global, calculated data base of shape-isomer properties is highly useful in developing models that take into account the isomer influence on reaction rates.

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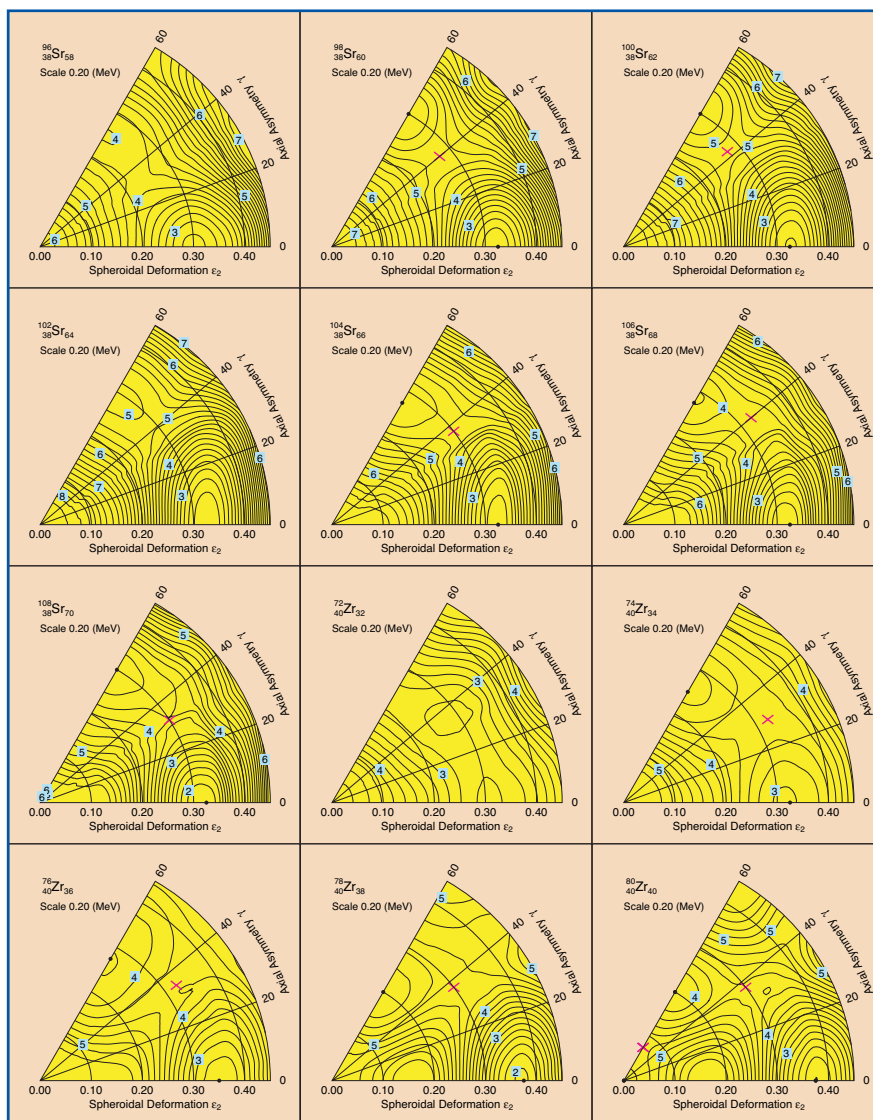


Figure 1—
Twelve calculated potential energy surfaces. Nine of the nuclei plotted have more than one minimum. The nucleus $^{80}\text{Zr}_{40}$ has one spherical minimum, one prolate minimum and one oblate minimum. Only minima deeper than 0.2 MeV are indicated.